Quantum Information and Quantum Computer

SS 2018 **5 . Exercise** **24.05.2018**

Task 1

A problem when solving the time-dependent Schrödinger equation on a grid is the preparation of the initial-state wave function $\psi(t_0 = t = 0)$. This applies especially, if the quantum algorithm discussed in the lecture should be used. Consider the specific example of the hydrogen atom which is initially in its electronic ground state and interacts later with a time-dependent electrical field (turned on at time $t_i > t_0$). Classically, you would project the known hydrogen ground-state wave function onto the grid in order to obtain $\psi(t_0)$. However, how can this wavefunction be implemented on a quantum computer? Also in this case a procedure known from the standard wave-packet propagation helps, the *propagation in imaginary time*. In fact, this procedure is also extremely helpful for finding the unknown ground state of a *time-independent* Hamiltonian.

a) Explain why the imaginary-time propagation, i. e. the substitution $t \rightarrow -i\,\tau$ (with the real numbers t, τ) followed by a "time propagation" in τ with the Hamiltonian $\hat{\mathrm{H}}$ yields the ground-state wave function ϕ_0 (with $\hat{\mathrm{H}}\,\phi_0 = E_0\,\phi_0$).

b) Show how it is possible to make use of the knowledge of the ground-state energy E_0 (for example in the above-mentioned example of the hydrogen atom) in the algorithm of imaginary-time propagation.

Task 2

Show that the operator

$$\hat{\sigma}_\psi \;=\; 2\,|\,\psi\,\rangle\langle\,\psi\,|\;-\;\hat{\mathrm{I}}$$

with the identity operator $\hat{\mathrm{I}}$ and the arbitrary vector $|\,\psi\,\rangle$ corresponds to a reflection on vector $|\,\psi\,\rangle$, i. e. the application of the operator $\hat{\sigma}_\psi$ on an arbitrary vector $|\,\phi\,\rangle$ results in a reflection of $|\,\phi\,\rangle$ on $|\,\psi\,\rangle$ in which the reflected vector lies in the plane formed by $|\,\psi\,\rangle$ and $|\,\phi\,\rangle$.

Task 3

Show that the Grover iteration operator $\hat{\mathrm{G}}$ represented in the $\{|\,\alpha\,\rangle, |\,\beta\,\rangle\}$ basis can be expressed as the rotation matrix

$$\mathbf{G} \;=\; \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \quad ,$$

if $\hat{\mathrm{G}} = (2\,|\,\psi\,\rangle\langle\,\psi\,| - \hat{\mathrm{I}})\hat{\mathrm{O}}$ holds where $\hat{\mathrm{I}}$ and $\hat{\mathrm{O}}$ are the identity and the oracle operator, respectively. The wavefunction ψ is the uniform superposition of all standard computer basis states,

$$|\,\psi\,\rangle \;=\; \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} |\,j\,\rangle \quad ,$$

with $N = 2^n$ where n is the number of qubits. On the other hand, $|\,\alpha\,\rangle$ is the (normalised) superposition of those basis states that do *not* correspond to any of the M hits. Analogously $|\,\beta\,\rangle$ is the (normalised) superposition of the M basis states characterizing hits. The oracle operator is defined in such a way that it multiplies the wavefunction describing the input state by a factor -1, if it corresponds to a hit.

Show also the validity of

$$\sin\theta \;=\; \frac{2\sqrt{M\,(N-M)}}{N}$$

and discuss the consequences, if the number of hits M lies in between $N/2$ and N.